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A SAFER ROUTE TO MDI, An assessment of a phosgene free manufacturing process

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2010

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):
Vetter, J. (2010). A SAFER ROUTE TO MDI, An assessment of a phosgene free manufacturing process. Groningen: s.n.

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Download date: 12-11-2019

Abstract

In this research the technological and economical feasibility of a new technology for the production of methylene diphenyl diisocyanate (MDI) is assessed.

Context

The global consumption of MDI totalled 4,150 kT in 2009 and an annual growth of 4.6% is expected until 2013. MDI is almost exclusively used for the production of polyurethane (PU). Currently the growth has stagnated due to the financial crisis, but it is still expected that this downfall is temporary, and that additional capacity investments are needed in the future.

At the moment all commercial MDI production technology is based on a phosgenation process. In this process phosgene is used as a feedstock component. Phosgene is a highly toxic gas and therefore causes major safety hazards. It is also a controversial material because it can, and has been used as a chemical warfare agent. Consequently phosgene using production processes are banned from many regions, especially the Middle East.

A lot of scientific research has been conducted on phosgene free production processes of MDI, though none of these processes has been commercialized. This study assesses the technological and the economical feasibility of the most viable phosgene free route to MDI. The studied route consists of three steps:

- The synthesis of methyl phenyl carbamate (MPC) from aniline and dimethyl carbonate (DMC) feedstock.
- MPC is condensed with formaldehyde to form dimethyl methylene diphenyl dicarbamate (MDC).
- MDC is thermally decomposed to MDI. Methanol is produced as a valuable by-product.

The major advantages of a phosgene free route to MDI are: (1) the process contains less safety hazards and (2) the availability of a competitive phosgene free route to MDI does comply with the strict regulations in all regions and thus create new business opportunities.

The research was initiated by Fluor; Fluor is a “Fortune 500” company that delivers engineering, procurement, construction, maintenance (EPCM), and project management to governments and clients in diverse industries around the world, including the PU industry. The research is intended for use in business development activities.

Goal

The goal of this research is to assess the process technologies and economics of a phosgene free production process of MDI in an effort to support a Fluor strategy for further development in these markets.

This goal has led to two main research questions:

1. Is it technologically feasible to produce phosgene free MDI on a commercial scale?
2. Is it economically feasible to produce phosgene free MDI on a commercial scale?

Conclusions - Technological feasibility

The studied phosgene free production process is technologically feasible but it still contains many uncertainties. Therefore additional research is necessary before the phosgene free technology can be implemented on a commercial scale. The most important uncertainties are the following.

1. The actual reaction performance of all three synthesis reactions on a large scale.
2. The quality and functionality of the produced MDI.
3. The physical properties of all process components.
4. The separation of the DMC:methanol azeotrope.

Based on these conclusions, four steps are necessary to develop a proven process that can be up scaled to a production plant of commercial scale:

1. The physical properties and process behaviour of many components need to be investigated.
2. A reliable catalyst system for each reaction needs to be developed.
3. A separation method for the DMC:methanol azeotrope needs to be developed.
4. A pilot plant needs to be set up to prove and optimize the process.

Conclusions - Economical feasibility

The currently available phosgene free MDI production technology is economically inferior to the conventional technology. The new technology does need financial investments, but the current financial situation, with low MDI prices, is not an incentive for additional capacity investments. Moreover, the currently installed production capacity of MDI is expected to be sufficient to meet the global demand until 2013 at least. Regardless of the financial crisis, growths in the MDI markets are still expected.

Even though the phosgene free technology is not competitive today, this study indicates that it does have the potential to become cost competitive. Governments and legislative institutions could impose stricter legislation and thereby stimulate the development of the phosgene free technology and enforce a transition in this market. This is a very plausible situation since the new technology can be cost competitive in comparison to the conventional technology and it does show significant improvements concerning HSE (Health, Safety, Environment). The polycarbonate case is similar to that of MDI and does confirm this sequence of events.

The phosgene free MDI production technology may eventually become economically feasible when future circumstances change, for instance if (1) stricter legislation is imposed, (2) the performance of the phosgene free process is improved and/or (3) if the DMC cost is decreased.

Path forward – Fluor

Phosgene free production of MDI is not expected to become reality in the near future and new MDI plants will probably still be based on the conventional phosgenation production process, unless there are significant improvements in the phosgene free technology or stricter governmental legislation is imposed that would restrict the phosgene using MDI production technology and enforces alternative technologies. The latter case is not unlikely as it happened before in the similar polycarbonate technology.

For Fluor this implicates that there are multiple options possible; which range from an active to a proactive stance.

The active stance means that no immediate action is taken. The situation and developments in the MDI market will be monitored and if the business environment changes, i.e. due to technological breakthroughs or stricter governmental regulations, Fluor can act accordingly. As long as the status quo is maintained, business is continued as usual.

The proactive stance implies that Fluor will interfere in the discussion by actively promoting the development of the phosgene free MDI production technology. Promotion can be done by, for example, publishing articles that support the development of the new technology or collaborating with public or private research institutions to increase scientific progress in this field. In this way it could accelerate a transition to a new production technology in the MDI markets. By finding strategic partners and be directly involved in new developments, this option could result in Fluor being a frontrunner in an emerging market of phosgene free MDI production.

Fluor has a very active policy concerning HSE; therefore the proactive stance would be in line with the company's strong sense of global responsibility and could even strengthen the position of Fluor in this field. However, Fluor is also a public owned company and therefore focused on profits; active involvement in the development of this new technology will consume resources and it is not certain whether it will be profitable. A trade-off has to be made between the degree of involvement and the amount of resources that Fluor is willing to dedicate to the development of a phosgene free MDI production technology.

Path forward – Scientific community

Phosgene free MDI production is not economically viable based on the current knowledge. However, this research does show that the cost of the described phosgene free process is similar to that of the conventional process. Moreover, there is definitely a cost competitive potential; especially if legislation is enforced to accelerate the development of the phosgene free MDI production technology. The major disadvantage of the technology is that the described phosgene free process is new and therefore contains many uncertainties, as opposed to the fully developed conventional production process.

As described in the 'Conclusions - Technological feasibility' paragraph above, there are four major steps necessary to develop a proven process for phosgene free MDI production. These steps serve as recommendations for further research and can be addressed by the scientific community.

However, to utilize the economical potential of the new technology, it does not only need to be proven but it does need improvement. Therefore more concrete targets for experimental research are set. These targets are derived from the economical feasibility study. Reaching these targets would significantly improve the competitive position of the phosgene free technology. The targets are the following.

- The amount of nitrobenzene needed has to be decreased by at least 50%.
- The reaction performance of the MPC synthesis reaction has to be improved; (1) the DMC:aniline ratio needs to be decreased from 7:1 to 2:1 and (2) the residence time of 8 hours needs to be decreased in order to minimize the reactor volume.